VALIDATION OF WATER QUALITY PARAMETERS RETRIEVED FROM INVERSE MODELING

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## 1. INTRODUCTION

Understanding the relationship between reflectance, absorption and backscattering of water is essential for developing the analytical and multitemporal algorithms necessary to use remote sensing as a management tool in the estuarine/coastal environment. The objective of this paper is to demonstrate utility of bio-optical modeling and retrieval techniques to derive the concentrations of important water properties (chlorophyll, color dissolved organic matter, etc.). This is a prerequisite to retrieve water quality parameters from the AVIRIS data acquired in July 13th 2001 over the Hudson/Raritan Estuary of NY-NJ. Atmospheric correction algorithm, coupled atmosphere ocean (CAO) system based on discrete ordinate method (DISORT) is applied to compensate for the atmospheric effects and to infer the water-leaving radiance. We used the linear matrix inversion model developed by Hoge and Lyon (1996) for retrieval of the inherent optical properties (IOPs) from which the water constituent concentrations are obtained. Validation was performed using the insitu measurements collected simultaneously with the AVIRIS overflight.

The study area is the Hudson/Raritan Estuary located south of the Verrazano Narrows and bordered by western Long Island, Staten Island and New Jersey (figure 1) Fresh water flows into the estuary mainly from the Hudson and Raritan Rivers and ocean waters enter tidally across the Sandy

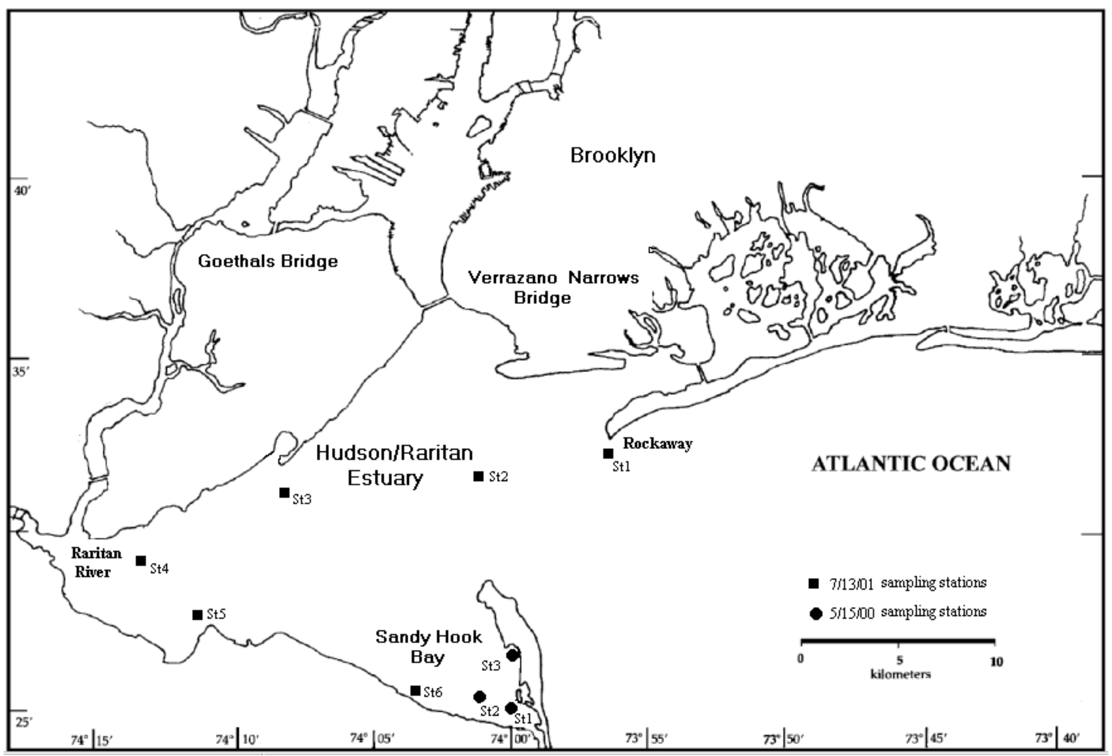


Figure 1. Map of the study area and locations of the sample points surveyed on 7/13/01

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Hook-Rockaway transect. The tidal water is mixing with fresh water inflows, in highly dynamic environments where there are major conflicting interests on the use of these waters. This shallow (< 8 m) and eutriphicated interface of the Hudson and Raritan Rivers and Atlantic Ocean was cruised during the field seasons in 1998-2001 with RV Walford and Blue Sea (MAST).

## 2. RESEARCH MATERIALS AND METHODS

### 2.1 AVIRIS

On July 13th, 2001, the AVIRIS, was flown over the study area. The AVIRIS images the earth's surface in 224 spectral bands approximately 10 nm wide covering the region 400-2500 nm from a NASA ER-2 aircraft at an altitude of 20 km. The ground resolution is 20m*20m. A geometric correction algorithm is applied to the AVIRIS data for correlation with in situ measurements. Atmospheric correction is required for retrieval of the inherent optical properties (IOPs) from which the water constituent concentrations are obtained.

### 2.2 Spectroradiometer

An OL 754 scanning, submersible spectroradiometer was deployed at six sampling stations as marked in figure1 simultaneously with the AVIRIS overflight. It uses a double monochromator for low stray light and measures spectral data from 300 nm to 850 nm. Upwelling ($E_u(\lambda)$) and downwelling ($E_d(\lambda)$) irradiances are measured and used to calculate the subsurface irradiance reflectance R(0-) for comparison with modeled reflectances. Figure 2 depicts the reflectance spectra recorded by the OL-754 at stations 2-6 on Jul. 13$^{th}$, 2001. (Note that the reflectance data from Station 1 is not included due to pronounced effect of wave propagation.)

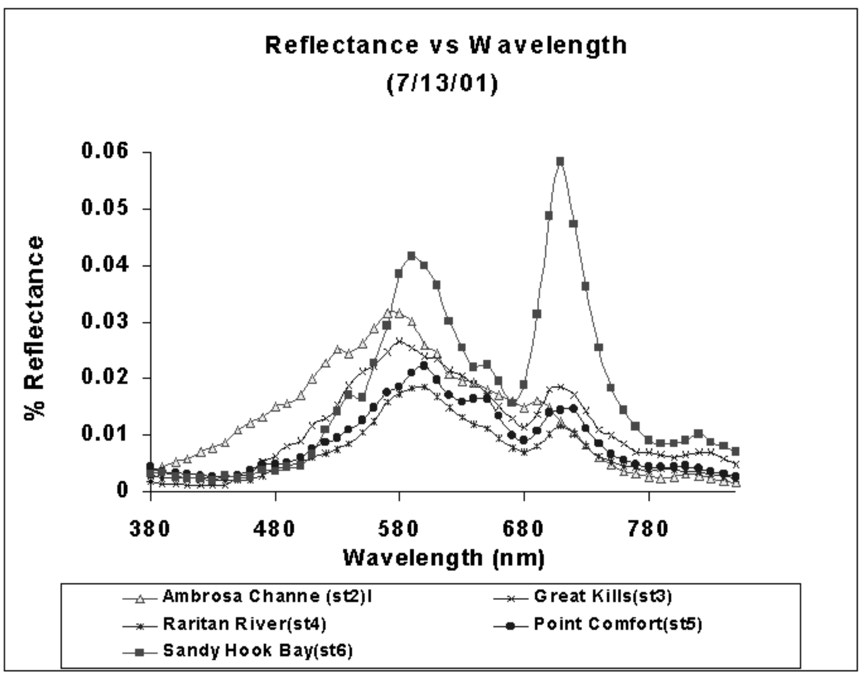



Figure 2. The reflectance spectra recorded by the OL-754 at designated sampling stations

### 2.3 Attenuation-absorption meter

Measurements of spectral absorption and beam attenuation coefficients were made using the ac-9 instrument. The ac-9, with one absorption flow tube and one attenuation flow tube, measures beam absorption (a) and attenuation (c) coefficient at 9 wavelengths (412, 440, 488, 510, 532, 555, 650, 676, 715 nm). The scattering coefficient (b) is obtained from a and c, since b = c - a. Use of the ac-9 has enabled us to model the backscattering coefficient ($b_b$), which is an important input parameter for establishing the IOPs of the estuary (in preparation). Figure 3 shows the absorption spectra recorded by the ac-9 at station 5 (Point Comfort) on July 13, 2001.

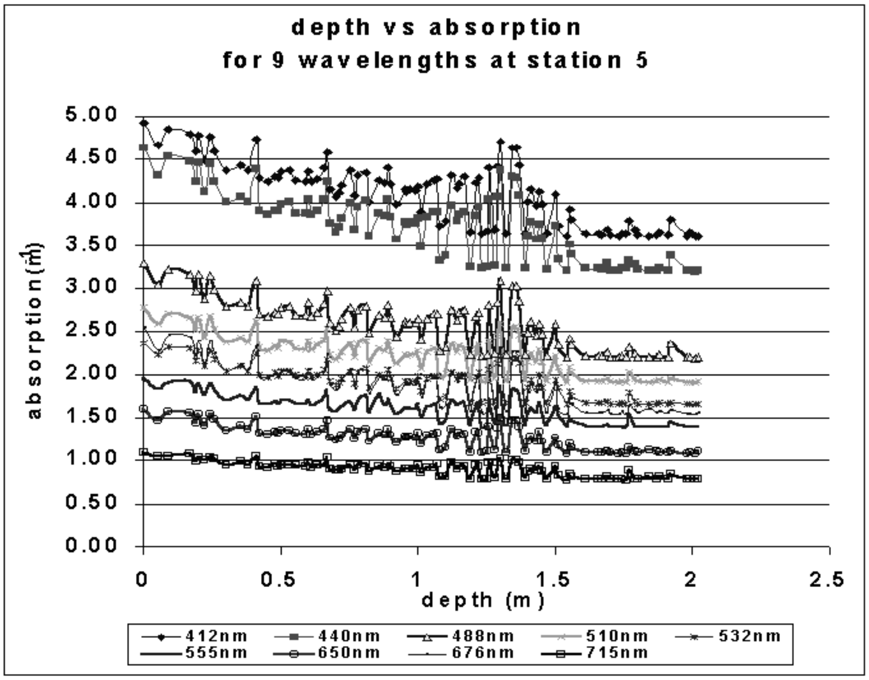



Figure 3. The absorption spectra for 9 wavelengths recorded by the ac-9 at station 5

### 2.4 Shipboard sampling

Water samples were collected (0.2 to 0.5 m depth) from selected sample stations as marked in figure 1 for laboratory analysis. Standard procedures were used to determine the concentrations of total chlorophyll_a (TCHL) (as indication of concentration of phytoplankton) and total suspended matter (TSM) (NEN 6520 (1981)) and NEN 6484 (1982)) respectively. The samples were analyzed for their IOPs as well as the identification/enumeration of the phytoplankton species. This was done to demonstrate the variety and composition of phytoplankton populations for input into library spectra of the estuary, which is currently in progress (Bagheri et al., 1999). The most abundant organisms identified were the Diatoms; Skeletonema sp. in high/moderate counts (7520-540 cells/ml). Also present in low counts were Flagellates; Eutreptia sp. (60 cells/ml) and Prorocentrum minimum (60 cells/ml). The TCHL concentrations varied between 73mg $m^{-3}$ and 17 mg $m^{-3}$ indicating that the measurements did not coincide with any major outbreaks of phytoplankton blooms. Likewise, the TSM ranges (23-5 g $m^{-3}$) were within the expected values for the time of year when the measurements taken.

## 3. DATA ANALYSIS and MODEL DEVELOPMENT

### 3.1 Atmospheric correction of the AVIRIS data

The remote sensing signal received by the AVIRIS is the sum of the water-leaving radiance and contribution from atmospheric aerosols and molecules. Comparison of the AVIRIS measured radiance and in-situ reflectance measurements reveals the effect of the atmosphere on the total upwelling spectral radiance measured by AVIRIS (Green et al., 1996). In atmospheric correction, the most challenging issue is to remove the impact of the highly variable aerosol component on top of the atmosphere (TOA) to convert remote sensing measured radiance into normalized water leaving radiance. This is the required input to algorithms designed to retrieve phytoplankton pigments or suspended solid concentrations. The aim is to calibrate the AVIRIS data spectrally and radiometrically to radiance/reflectance for bio-optical and inverse modeling and generation of thematic maps of water quality parameters. We use a comprehensive radiative transfer model for the coupled atmosphere-ocean (CAO) system based on the discrete-ordinate method (DISORT) to compute the radiance within and backscattered from the atmosphere-ocean system (Jin and Stamnes, 1994; Thomas and Stamnes, 1999). This CAO-DISORT model, in which multiple scattering by ocean particles are properly treated, is also suitable for constructing an atmospheric correction algorithm (Stamnes et al., 2002), and it can be used to calculate the amount of light incident above the water surface (downwelling irradiance) for a given geographic location and a chosen atmosphere.

Algorithms for retrieving the chlorophyll concentration from space have been developed for sensors such as CZCS (coastal Zone Color Scanner), SeaWiFS (the Sea-viewing Wide Field-view Sensor), MODIS (the Moderate-Resolution Imaging Spectroradiometer) and others. However, most of these algorithms have been applied mainly to the case I water. These algorithms usually include two steps. The first step is atmospheric correction, which is applied to separate the atmospheric radiance from the radiance that comes from the ocean. The next step is based on a bio-optical model to relate the water-leaving radiance to the chlorophyll concentration. Because the water-leaving radiance typically comprises at most about 10% of the total radiance at the TOA, the key to reliable retrieval of the water-leaving radiance from the measured total radiance is an accurate correction of the effects of aerosol scattering and absorption.

Based on the CAO-DISORT radiative transfer model for the coupled atmosphere-ocean system (CAO-DISORT, Stamnes et al., 1988; Jin and Stamnes, 1994; Thomas and Stamnes, 1999) and a complete bio-optical model of Case I waters (Li and Stamnes, 2002), we have developed a new algorithm for SeaWiFS data processing (Stamnes et al., 2002). The CAO-DISORT code computes multiple scattering effects in a rigorous manner, and automatically and accurately takes into account the anisotropic behavior of the water-leaving radiance. The SeaWiFS channels 765 nm and 865 nm are used for retrieval of aerosol optical depth and aerosol model due to the small contribution from the case I water in the NIR. Then, the retrieved aerosol model and optical depth are used to predict the water leaving radiance in the visible, and subsequently to retrieve the chlorophyll concentration from the SeaWiFS channels at 490 nm and 555 nm. This approach provides simultaneous retrieval of atmospheric aerosol properties and chlorophyll concentrations in Case I waters. This new algorithm has been tested on synthetic datasets as well as match-up data. The results show that our new algorithm provides self-consistent and accurate retrievals.

Now this algorithm is being modified for use with the AVIRIS data to retrieve marine parameters for coastal waters. The AVIRIS data should be ideal for coastal water retrieval due to the many spectral channels available, and the wide spectral range from 400 nm to 2500 nm. The channels at 765 nm and 865 nm are no longer suitable for aerosol retrieval in the coastal water, because of the strong scattering of coastal water. The longer wavelength channels, such as 1040 nm and 1240 nm, will be selected to retrieve aerosol properties. In contrast to Case I waters where the optical properties are assumed to covary with the chlorophyll concentration, a bio-optical model for coastal waters must include other parameters. At a minimum we should include 3 different components: chlorophyll (CHL), color dissolved organic matter (CDOM) and total suspended solids (TSM). Because the different components have different spectral scattering/absorption characteristics, the wide spectral range of the AVIRIS instrument provides a good opportunity for retrieval of multiple components. Feasibility studies based on a three-component model (Frette et al., 1998; Frette et al., 2001) show promising results. Based on the field measurements obtained over the Hudson/Raritan Estuary area (Bagheri et al., 1999, 2000 and 2001). We have used a three-component bio-optical model in conjunction with the CAO-DISORT code to compute the radiance both at the surface and at the top of the atmosphere. Figure 4 shows comparison of reflectances measured and computed from CAO-DISORT code using a bio-optical model consistent with the measurements.

Building such bio-optical models for special coastal locations will be very important step for developing reliable algorithms to retrieve the coastal water parameters. The high spatial resolution of the AVIRIS data will also be very advantageous for coastal water property retrieval, because coastal waters usually have high spatial and temporal variation. Thus, the AVIRIS data has suitable resolution data for coastal water quality estimation.

### 3.2 Bio-Optical and Inverse Modeling

The ongoing research is based on imaging spectrometer data from AVIRIS, field spectroradiometer and water samplings. Based on these measurements optical water quality models are constructed linking the water constituent concentrations to (i) the inherent optical properties (IOP), using the specific inherent optical properties (SIOP), and (ii) to the subsurface (ir)radiance reflectance (Bagheri and Dekker , 1999 and Bagheri et al., 2000 and 2001).

The subsurface irradiance reflectance R(0-) are generated from the constituent concentrations using the linear backscattered albedo model based on the work of Gordon et al. (1975):

$$R(0-) = r \cdot \frac{b_b}{a + b_b} \qquad (1)$$

Where:

a is the total absorption coefficient

$b_b$ is the total scatter coefficient

r is a factor based on the geometry of incoming light and volume scattering in the water body.

This model is then validated with the R(0-) measured in the study site (figure 4). The validation of subsurface irradiance reflectance measured by the spectroradiometer is an important step for establishing the optical properties of the waters of the study site. Modeling of reflectance spectra based on the IOP will explain the variability in water quality concentrations and inverse modeling can be used for monitoring water quality conditions in the estuarine waters using remotely sensed data.

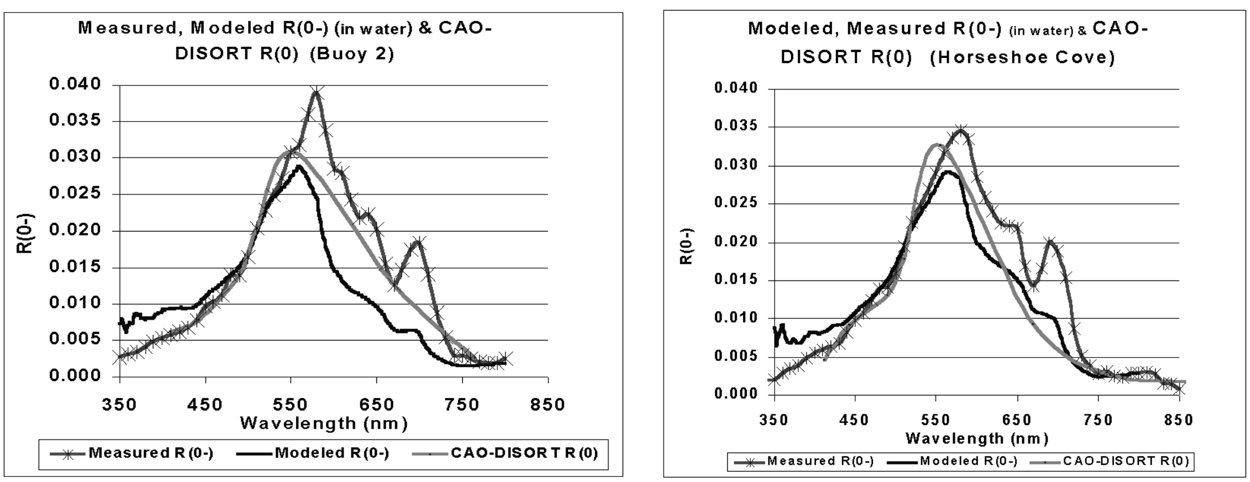



Figure 4. Modeled, Measured R(0-) and CAO-DISORT R(0) computed for Stations 2&3 (5/15/2000)

The linear matrix inversion developed by Hoge et al. (1996) was applied to in situ measurements collected simultaneously with the AVIRIS overflight. The radiance models describe the generation of upwelled water-leaving spectral radiance caused by backscatter and absorption of incident downwelling solar irradiance (Hoge et al., 2001). The algorithm was then applied to the atmospherically corrected AVIRIS data acquired over the study area to retrieve the IOPs (from which the constituent concentration are obtained). The linear matrix inversion for retrieval of IOPs was based on the work of Gordon et al. (1988).

The inversion matrices (2) are used for solving for three unknown $a_{ph}(\lambda_1)$, $a_d(\lambda_1)$ and $b_{bt}(\lambda_1)$ at any wavelength $\lambda_i$:

$$\begin{bmatrix} 1 & 1 & v(\lambda_1) \\ D_{21} & e^{[-S(\lambda_2-\lambda_1)]} & (\lambda_1/\lambda_2)^n v(\lambda_2) \\ D_{31} & e^{[-S(\lambda_3-\lambda_1)]} & (\lambda_1/\lambda_3)^n v(\lambda_3) \end{bmatrix} \cdot \begin{bmatrix} a_{ph}(\lambda_1) \\ a_d(\lambda_1) \\ b_{bt}(\lambda_1) \end{bmatrix} = \begin{bmatrix} h(\lambda_1) \\ h(\lambda_2) \\ h(\lambda_3) \end{bmatrix} \tag{2}$$

where:

$\lambda_1 = \lambda_g$----peak wavelength for Gaussian phytoplankton absorption model (nm)

$\lambda_1$=440, $\lambda_2$ = 500, $\lambda_3$ =560 nm

S = 0.025, n = 1.2, g = 30

V--- a factor to separate absorption and scattering components of water

$$D_{21} = e^{(\lambda_2-\lambda_1)^2/-2g^2} \qquad D_{31} = e^{(\lambda_3-\lambda_1)^2/-2g^2}$$

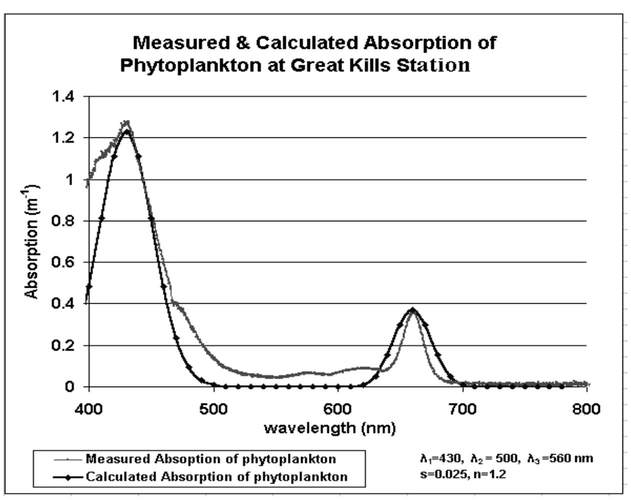
The $a_{ph}(\lambda_i)$, $a_d(\lambda_i)$ and $b_{bt}(\lambda_i)$ at all wavelengths are computed using the following:

$$a_{ph}(\lambda_i) = a_{ph}(\lambda_g) \cdot e^{[(\lambda_i-\lambda_g)^2/(-2g^2)]} \tag{3}$$

$$a_d(\lambda_i) = a_d(\lambda_d) \cdot e^{[-s(\lambda_i-\lambda_g)]} \tag{4}$$

$$b_{bt}(\lambda_i) = b_{bt}(\lambda_b)(\lambda_b/\lambda_i)^n \tag{5}$$

The results of the linear matrix inversion were input into Equation (1)-- the bio-optical model of the estuary for retrieval of water quality parameter concentration (figure 5).



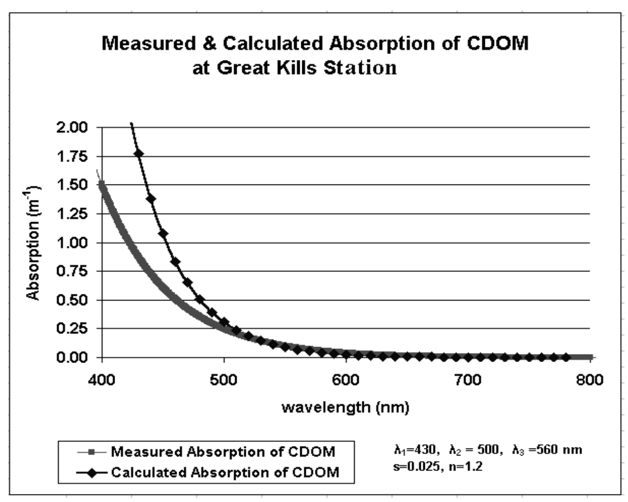




Figure 5. Measured and Retrieved Phytoplankton and CDOM absorptions at Great Kills (St 3) (7/13/2001)

## 4. DISCUSSION AND CONCLUSION

Atmospheric correction of ocean color imagery is commonly based on the assumption that the water-leaving radiances at NIR are negligible. Over the open ocean an aerosol model and aerosol optical depth can be derived from the NIR channels. The aerosol information can be extrapolated into the visible range for retrieval of the water leaving radiance and the estimation of the chlorophyll concentration. Unfortunately, these algorithms cannot be used in case 2 waters because the suspended material in case 2 waters have strong scattering in the NIR part of the spectrum. Development of a robust algorithm for simultaneous retrieval of atmospheric aerosol optical properties, chlorophyll concentration and colored dissolved organic matter is a very challenging task. Nevertheless, such an algorithm is needed to make progress in this area.

The AVIRIS is capable of measuring hydrologic optical properties at a level of detail unmatched by any existing satellite instrument. The AVIRIS hyperspectral data provide us with an opportunity to develop such algorithms based on the different spectral reflectances characterizing aerosol and ocean particles. This can be used as a basis for distinguishing between atmospheric and oceanic effects and to set the estimated turbidity for each region within the image for retrieval of water constituents. The methodology described here provides a baseline for better understanding of how sunlight interacts with estuarine/coastal water necessary in establishing the IOP characterization of the estuary and setting a foundation for the future research. The products of remote sensing data derived from AVIRIS analysis in forms of thematic maps representing the spatial/temporal distributions of water quality parameters are important input into a GIS for better management of the water resources of the study site and other estuaries nationwide.

## 5. ACKNOWLEDGEMENT

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## 6. REFERENCES

Bagheri, S., and Dekker, A., 1999, Remote Sensing of Nearshore Water Quality Using Bio-Optical Modeling and Retrieval Techniques, *8th AVIRIS Workshop*. Pasadena, California.

Bagheri, S., Zetlin, C., and Dios, R., 1999, Estimation of optical properties of nearshore water, *International Journal of Remote Sensing*, Vol. 20, No. 17, 3393-3397.

Bagheri, S., Rijkeboer, M., Pasterkamp, R., and Dekker, 2000, A Comparison of Field Spectroradiometers in Preparation of Bio-Optical Modeling, *9th JPL AVIRS Workshop*. Pasadena, California.

Bagheri, S., and Stamnes, K and Li, W., 2001, Application of Radiative Transfer Theory to Atmospheric Correction of AVIRIS Data, *10th JPL AVIRS Workshop*. Pasadena, California.

Frette, O., Stamnes, J. J., and Stamnes, K., 1998, Optical remote sensing of marine constituents in coastal waters: A feasibility study, *Applied Optics*, 37, 8218-8326.

Frette, O., Erga, S. R., Stamnes, J. J., and Stamnes, K., 2001, Optical remote sensing of waters with vertical structure, *Applied Optics*, 40, 1478-1487.

Gordon, H. R., Brown O. B., and Jacobs, M. M., 1975, Computed Relationships between Inherent and Apparent Optical Properties of a Flat Homogeneous Ocean. *Appl. Optics*, 14:417-427.

Gordon, H. R., Brown, O. B., Evans, R. H., Brown, J. W., Smith, R. C., Baker, K. S., and Clark, D. K., 1988, A semianalytic radiance model of ocean color, *J. Geophys. Res.*, 93, 10,909-10,924.

Green, R. O., 1996, Summaries of the 6th Annual JPL Airborne Earth Science Workshop. Vol. 1, *JPL AVIRIS Workshop*. Pasadena, California.

Hoge, F. E., and Lyon, P.E., 1996, Satellite retrieval of inherent optical properties by linear matrix inversion of oceanic radiance models: An analysis of model and radiance measurement errors, *J. Geophys. Res.* 101, 16,631- 16,648.

Hoge, F.E., Wright, C. W., Lyon, P.E., Swift, R. N., and Yungel, J.K., 2001, Inherent optical properties imagery of the western North Atlantic Ocean: Horizontal spatial variability of the upper mixed layer, *J. Geophys. Res.* 106, 31129-31140.

Jin, Z., and Stamnes, K., 1994, Radiative transfer in nonuniformly refracting media such as the atmosphere/ocean system, *Appl. Opt.*, 33, 431-442.

Li, W., and Stamnes, K., 2002, Inherent optical properties of case I waters: A complete model suitable for use in radiative transfer computations, *J. Geophys. Res.*, submitted.

NEN 6484, 1982, Water: Determination of the content of not dissolved material and its ignition residue, *Nederlands Normalisatie instituut, Delft, The Netherlands (in Dutch)*

NEN 6520, 1981, Water: Spectrophotometric determination of chlorophyll a content, *Nederlands Normalisatie instituut, Delft, The Netherlands (in Dutch)*

Stamnes, K., Tsay, S.-C., Wiscombe, W.J. and Jayaweera, K., 1988, Numerically stable algorithm for discrete-ordinate-method radiative transfer in multiple scattering and emitting layered media, *Appl. Opt.* 27, 2502-2509.

Stamnes, K., Li, W., Yan, B., Barnard, A., Pegau, W. S., and Stamnes, J. J., 2002, A new ocean color algorithm: Simultaneous retrieval of aerosol optical properties and chlorophyll concentrations, *Appl. Optics,* submitted.

Thomas, G. E., and Stamnes, K., 1999, Radiative Transfer in the Atmosphere and Ocean, *Cambridge University Press.*